



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:29 PM UTC

PDB ID : 7EVN / pdb_00007evn
EMDB ID : EMD-31330
Title : The cryo-EM structure of the DDX42-SF3b complex
Authors : Zhang, X.; Zhan, X.; Shi, Y.
Deposited on : 2021-05-21
Resolution : 2.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

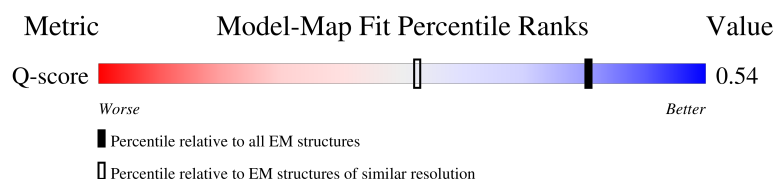
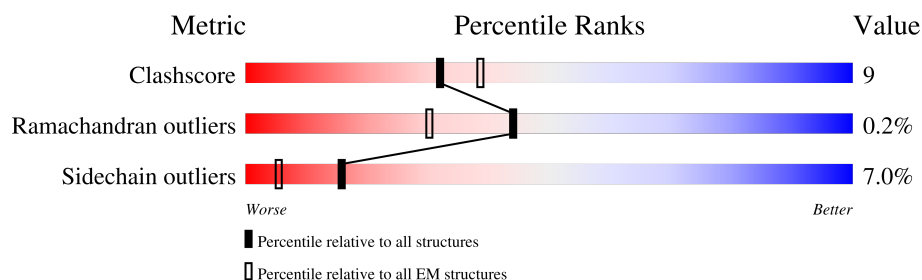
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	86	80% 8% • 9%
2	C	872	69% 23% • 7%
3	D	110	5% 75% 9% • 15%
4	A	1250	5% 73% 19% • 6%

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Mol	Chain	Length	Quality of chain
5	E	958	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19668 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	78	Total	C	N	O	S	0	0
			646	409	114	118	5		

- Molecule 2 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	815	Total	C	N	O	S	0	0
			6487	4163	1121	1164	39		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	433	MET	-	initiating methionine	UNP O75533
C	434	ALA	-	expression tag	UNP O75533
C	435	SER	-	expression tag	UNP O75533
C	436	ASP	-	expression tag	UNP O75533
C	437	TYR	-	expression tag	UNP O75533
C	438	LYS	-	expression tag	UNP O75533
C	439	ASP	-	expression tag	UNP O75533
C	440	ASP	-	expression tag	UNP O75533
C	441	ASP	-	expression tag	UNP O75533
C	442	ASP	-	expression tag	UNP O75533
C	443	LYS	-	expression tag	UNP O75533
C	444	ALA	-	expression tag	UNP O75533
C	445	SER	-	expression tag	UNP O75533
C	446	ASP	-	expression tag	UNP O75533
C	447	GLU	-	expression tag	UNP O75533
C	448	VAL	-	expression tag	UNP O75533
C	449	ASP	-	expression tag	UNP O75533
C	450	ALA	-	expression tag	UNP O75533
C	451	GLY	-	expression tag	UNP O75533

- Molecule 3 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	93	Total	C	N	O	S	0	0
			700	429	123	135	13		

- Molecule 4 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1177	Total	C	N	O	S	0	0
			9227	5858	1568	1756	45		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-32	TRP	-	expression tag	UNP Q15393
A	-31	SER	-	expression tag	UNP Q15393
A	-30	HIS	-	expression tag	UNP Q15393
A	-29	PRO	-	expression tag	UNP Q15393
A	-28	GLN	-	expression tag	UNP Q15393
A	-27	PHE	-	expression tag	UNP Q15393
A	-26	GLU	-	expression tag	UNP Q15393
A	-25	LYS	-	expression tag	UNP Q15393
A	-24	GLY	-	expression tag	UNP Q15393
A	-23	GLY	-	expression tag	UNP Q15393
A	-22	GLY	-	expression tag	UNP Q15393
A	-21	SER	-	expression tag	UNP Q15393
A	-20	GLY	-	expression tag	UNP Q15393
A	-19	GLY	-	expression tag	UNP Q15393
A	-18	GLY	-	expression tag	UNP Q15393
A	-17	SER	-	expression tag	UNP Q15393
A	-16	GLY	-	expression tag	UNP Q15393
A	-15	GLY	-	expression tag	UNP Q15393
A	-14	SER	-	expression tag	UNP Q15393
A	-13	ALA	-	expression tag	UNP Q15393
A	-12	TRP	-	expression tag	UNP Q15393
A	-11	SER	-	expression tag	UNP Q15393
A	-10	HIS	-	expression tag	UNP Q15393
A	-9	PRO	-	expression tag	UNP Q15393
A	-8	GLN	-	expression tag	UNP Q15393
A	-7	PHE	-	expression tag	UNP Q15393
A	-6	GLU	-	expression tag	UNP Q15393
A	-5	LYS	-	expression tag	UNP Q15393
A	-4	GLY	-	expression tag	UNP Q15393
A	-3	SER	-	expression tag	UNP Q15393
A	-2	ALA	-	expression tag	UNP Q15393

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP Q15393
A	0	ALA	-	expression tag	UNP Q15393

- Molecule 5 is a protein called ATP-dependent RNA helicase DDX42.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	486	Total	C	N	O	S	0	0
			2605	1555	505	542	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP Q86XP3
E	-18	ALA	-	expression tag	UNP Q86XP3
E	-17	SER	-	expression tag	UNP Q86XP3
E	-16	ASP	-	expression tag	UNP Q86XP3
E	-15	TYR	-	expression tag	UNP Q86XP3
E	-14	LYS	-	expression tag	UNP Q86XP3
E	-13	ASP	-	expression tag	UNP Q86XP3
E	-12	ASP	-	expression tag	UNP Q86XP3
E	-11	ASP	-	expression tag	UNP Q86XP3
E	-10	ASP	-	expression tag	UNP Q86XP3
E	-9	LYS	-	expression tag	UNP Q86XP3
E	-8	ALA	-	expression tag	UNP Q86XP3
E	-7	SER	-	expression tag	UNP Q86XP3
E	-6	ASP	-	expression tag	UNP Q86XP3
E	-5	GLU	-	expression tag	UNP Q86XP3
E	-4	VAL	-	expression tag	UNP Q86XP3
E	-3	ASP	-	expression tag	UNP Q86XP3
E	-2	ALA	-	expression tag	UNP Q86XP3
E	-1	GLY	-	expression tag	UNP Q86XP3
E	0	THR	-	expression tag	UNP Q86XP3

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	D	3	Total	Zn	0
			3	3	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

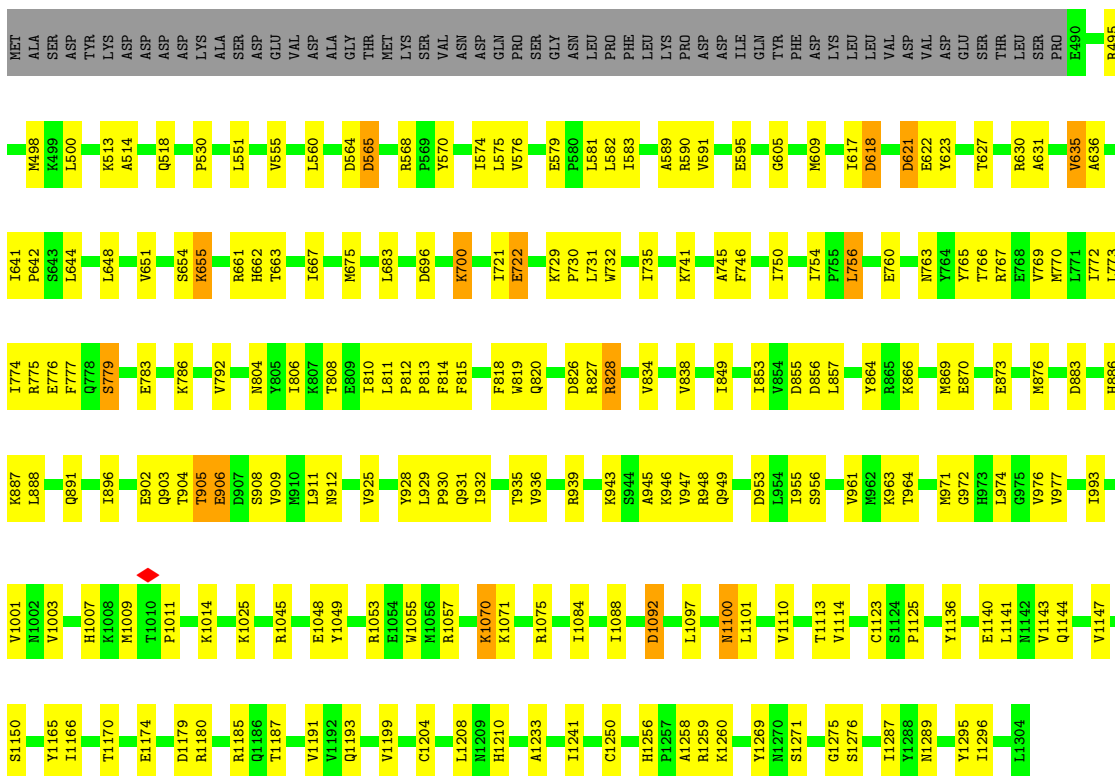
- Molecule 1: Splicing factor 3B subunit 5

Chain B: 



- Molecule 2: Splicing factor 3B subunit 1

Chain C: 

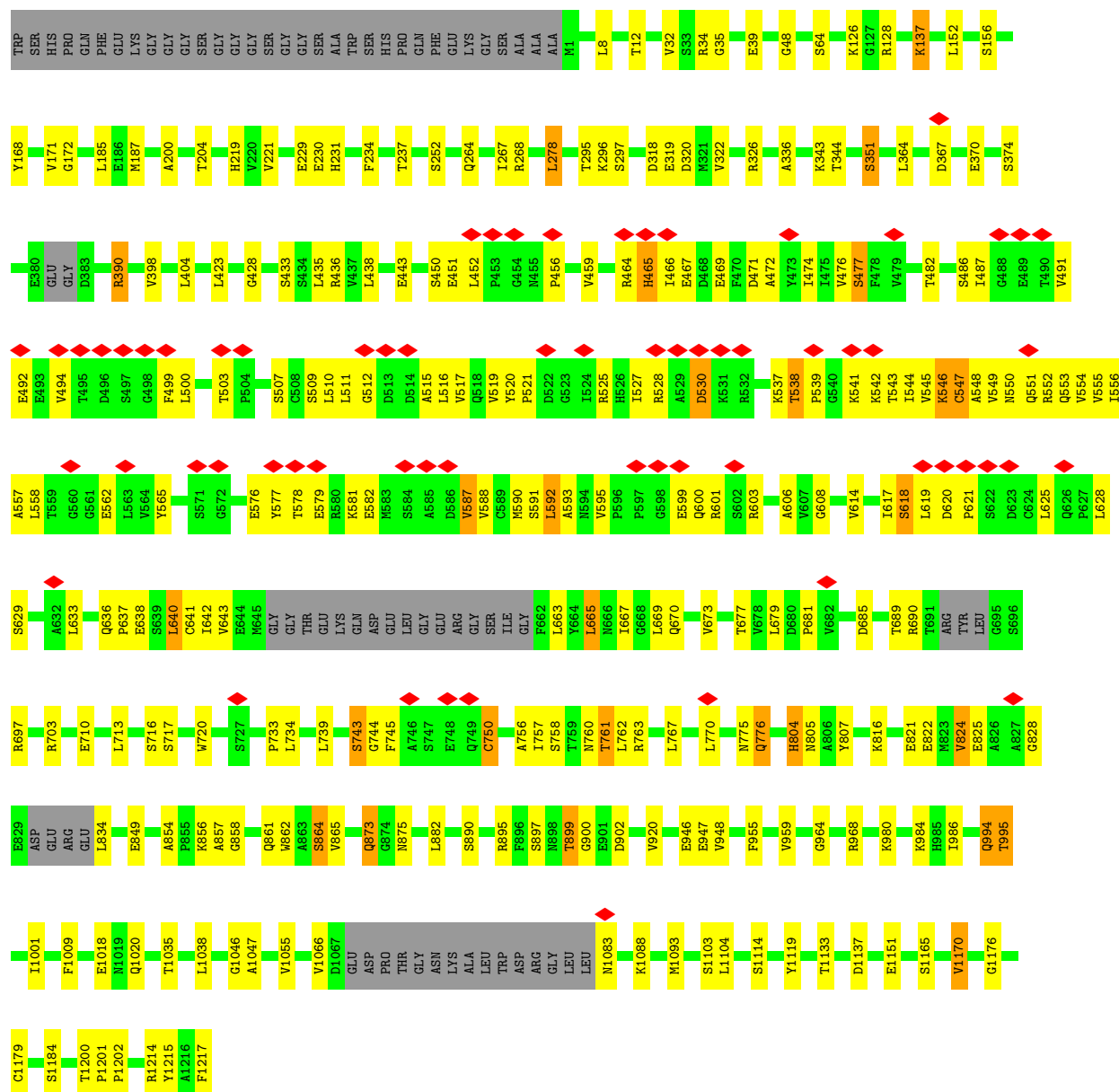
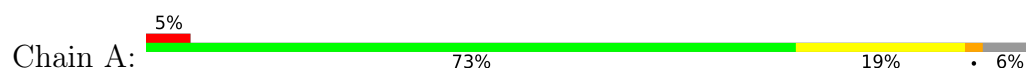


- Molecule 3: PHD finger-like domain-containing protein 5A

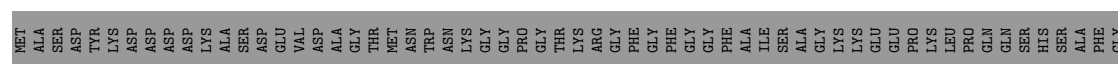
Chain D: 



• Molecule 4: Splicing factor 3B subunit 3



• Molecule 5: ATP-dependent RNA helicase DDX42



PRO	LYS	ARG	GLY	THR	THR	ASN	LEU	A598	N538	L478	E418	V358	K298	K238	GLU	ALA
LYS	MET	GLY	GLY	PRO	PRO	GLN	GLY	Y599	K639	H479	Y419	A359	T299	L239	ASP	THR
PRO	PRO	ASP	GLY	ALA	GLY	LYS	ARG	T600	V640	S480	Q420	V360	G300	M240	ASN	THR
VAL	VAL	TYR	GLY	ALA	GLY	GLY	ARG	L601	I641	G481	V421	Y361	S301	L241	LEU	SER
ASP	ASP	ARG	GLN	PRO	PRO	ALA	PRO	L602	S642	P482	R422	G362	G302	R242	TYR	SER
ASP	ASP	ARG	GLN	ALA	GLY	ALA	GLY	T603	D643	S483	S423	G363	K303	V243	ASP	GLY
SER	SER	HIS	VAL	VAL	VAL	GLY	GLY	P604	F644	K484	I424	G364	T304	S244	ASP	PHE
SER	SER	PRO	VAL	VAL	VAL	GLY	GLY	K605	K645	W485	A425	S365	A305	G245	GLY	LYS
MET	MET	LYS	GLU	ASN	ASN	ALA	LYS	D606	K646	N486	A426	A306	A306	G246	SER	LYS
ASP	ASP	SER	GLY	GLY	GLY	GLY	GLY	S607	K647	W487	H427	W367	F307	A247	PRO	ALA
LYS	LYS	SER	ASP	ALA	TRP	ASN	ASN	N608	D648	L488	V428	E368	I308	P248	ASP	PRO
VAL	VAL	ARG	THR	THR	THR	THR	ASP	F609	I649	T489	R429	Q369	W309	P249	GLN	PRO
ASP	ASP	HIS	GLY	GLY	GLY	GLY	ASP	A610	P650	R490	P430	K370	P310	L116	LEU	LEU
THR	THR	THR	ASN	ASN	ASN	ASN	GLY	G611	V651	R491	D431	K371	M311	P251	PRO	PRO
LYS	LYS	ASP	GLY	GLY	GLY	GLY	ASN	D612	L652	L492	R432	A372	L312	G252	PHE	PHE
ASP	ASP	HIS	ARG	ARG	ARG	ASN	ASN	L613	V653	V493	Q433	L373	I313	S253	TYR	TYR
LYS	LYS	ARG	GLY	GLY	GLY	VAL	VAL	V614	A554	E494	T434	Q374	H314	S254	LYS	LYS
ALA	ALA	GLY	THR	THR	THR	VAL	SER	R615	T655	F495	L435	E375	I315	F255	ILE	ILE
ASP	ASP	GLY	GLU	GLY	GLY	PRO	ASN	N616	D656	T496	L436	G376	M316	A256	SER	GLY
GLY	GLY	ASN	GLY	GLY	GLY	THR	THR	L617	V657	S497	F437	A377	D317	H257	LYS	LYS
PHE	PHE	ARG	GLY	SER	SER	ASN	GLU	E618	A658	S498	S438	E378	K318	F258	ARG	ARG
ALA	ALA	HIS	ALA	ALA	ALA	SER	ALA	G619	A659	G499	A439	I379	Q319	G259	ALA	ALA
VAL	VAL	GLY	GLY	GLY	GLY	GLN	TYR	R619	R660	S500	T440	V380	E320	F260	GLY	GLY
PRO	PRO	SER	ARG	ARG	ARG	GLN	PRO	A620	R661	S500	T440	V381	L321	D261	SER	SER
GLY	GLY	ALA	GLY	GLY	GLY	GLY	GLY	N621	G661	V501	F441	V381	L321	D261	ALA	ALA
PRO	PRO	GLY	ARG	ARG	ARG	HIS	THR	Q622	L662	L502	R442	C382	E322	E262	N68	N68
LYS	LYS	ARG	GLY	GLY	GLY	ASN	GLY	H623	D663	L503	K443	C383	P323	Q263	F69	F69
ARG	ARG	HIS	THR	THR	THR	SER	ALA	V624	I664	F504	K444	P384	G324	L264	D70	D70
LYS	LYS	GLY	GLY	GLY	GLY	PRO	MET	S625	P665	V505	I445	G385	D325	M265	E71	E71
LYS	LYS	GLY	GLY	GLY	GLY	ASP	GLY	S626	S666	T506	E446	R386	G326	H266	N73	N73
ARG	ARG	ARG	GLY	GLY	GLY	PRO	ARG	E627	I667	K507	K447	L387	P327	Q267	Y75	Y75
TRP	TRP	ALA	ALA	SER	SER	THR	THR	L628	K668	K508	L448	I388	I328	I268	F76	F76
ASP	ASP	ALA	ALA	ALA	ALA	SER	ALA	L629	T669	A509	A449	D389	A329	R269	E77	E77
LYS	LYS	ALA	LYS	LYS	LYS	ALA	MET	D630	V570	N510	R450	H390	V330	F217	D78	D78
ALA	ALA	GLY	ALA	ALA	ALA	LYS	ALA	L631	I571	A511	D451	V391	I331	V218	E79	E79
ASN	ASN	GLY	ALA	ALA	ALA	GLY	ALA	A632	N572	E512	I452	K392	V332	N219	E80	E80
GLY	GLY	GLY	ILE	PHE	PHE	ILE	PHE	M633	Y573	E513	L453	K393	C333	E220	E81	E81
THR	THR	THR	GLY	GLY	GLY	PRO	GLN	Q634	D574	L514	I454	K394	P334	H221	ASP	ASP
ASN	ASN	GLY	GLY	GLY	GLY	GLY	SER	Q635	V575	A515	D455	A395	T335	E222	SER	SER
GLY	GLY	ASN	ASN	ASN	ASN	PHE	GLN	A636	A576	N516	P456	T396	R336	E223	ASN	ASN
LYS	LYS	GLY	GLY	GLY	GLY	GLY	TYR	W637	R577	N517	I457	N397	E337	T224	VAL	VAL
HIS	HIS	HIS	HIS	HIS	HIS	ASN	LYS	F638	D578	L518	R458	L398	L338	T225	ASP	ASP
ASP	ASP	ASP	ASP	ASP	ASP	GLY	HIS	R639	I579	K519	V459	Q399	C339	N226	LEU	LEU
PRO	PRO	ARG	VAL	VAL	VAL	ILE	VAL	K640	D680	Q520	V460	R400	Q340	T227	PRO	PRO
GLY	GLY	HIS	ALA	ALA	ALA	GLY	ALA	S641	T681	Q521	Q461	V401	Q341	L227	ILE	ILE
LYS	LYS	GLY	ALA	ALA	ALA	GLY	ALA	R642	H682	G522	Q462	S402	I342	P228	PRO	PRO
MET	MET	GLY	SER	SER	SER	ALA	SER	F643	T683	H523	D463	Y403	H343	Q282	GLU	GLU
GLY	GLY	LEU	LEU	LEU	LEU	VAL	SER	LYS	N584	N524	I464	L404	A344	V284	ASN	ASN
									R685	L525	G465	V405	E345	P285	PRO	PRO
									L586	G526	E466	F406	C346	V286	THR	THR
									G687	L527	A407	A287	L288	R236	ARG	ARG
									R688	L528	ALA	E408	R348	L235	GLN	GLN
									T689	H529	ALA	A409	F349	H237		
									G590	G630	D470	D410	G350	G290		
									ARG	V471	V471	R291	K351	D292		
									ALA	T472	T472	M412	A352	D292		
									GLY	Q473	Q473	F413	M353	I294		
									E594	I474	I474	D414	K354	Q295		
									K595	V475	V475	M415	L355	I296		
									G596	E476	E476	G416	R356	A297		
									V697	R537	I477	F417	S357			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234800	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.235	Depositor
Minimum map value	-0.133	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	260.88, 260.88, 260.88	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	B	0.27	0/665	0.50	0/899
2	C	0.25	0/6609	0.48	2/8946 (0.0%)
3	D	0.29	0/709	0.47	0/952
4	A	0.27	1/9415 (0.0%)	0.46	1/12775 (0.0%)
5	E	0.62	0/2607	0.98	5/3593 (0.1%)
All	All	0.34	1/20005 (0.0%)	0.56	8/27165 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	804	HIS	C-O	6.55	1.32	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	275	GLN	CA-C-N	-8.04	111.73	119.85
5	E	275	GLN	C-N-CA	-8.04	111.73	119.85
5	E	271	SER	CA-C-N	6.98	134.27	121.70
5	E	271	SER	C-N-CA	6.98	134.27	121.70
2	C	565	ASP	N-CA-C	-5.91	104.74	113.61
2	C	564	ASP	O-C-N	-5.79	114.49	122.30
4	A	137	LYS	N-CA-CB	-5.49	107.91	114.17
5	E	462	GLY	N-CA-C	5.11	118.82	112.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	646	0	608	6	0
2	C	6487	0	6700	157	0
3	D	700	0	682	6	0
4	A	9227	0	9154	142	0
5	E	2605	0	1378	67	0
6	D	3	0	0	0	0
All	All	19668	0	18522	330	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (330) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:786:LYS:NZ	5:E:72:GLU:HG3	1.52	1.22
5:E:120:MET:HA	5:E:120:MET:HE2	1.24	1.18
2:C:741:LYS:HE3	5:E:79:GLU:HB2	1.19	1.15
4:A:221:VAL:CG1	5:E:146:GLY:HA3	1.82	1.10
2:C:741:LYS:CE	5:E:79:GLU:HB2	1.87	1.04
2:C:786:LYS:HZ1	5:E:72:GLU:HG3	0.87	1.01
2:C:662:HIS:CE1	2:C:700:LYS:HD2	1.95	1.00
2:C:630:ARG:NH2	5:E:68:ASN:HB2	1.79	0.97
5:E:162:ARG:HH11	5:E:162:ARG:HB3	1.27	0.96
5:E:162:ARG:HB3	5:E:162:ARG:NH1	1.82	0.94
5:E:120:MET:HA	5:E:120:MET:CE	2.00	0.91
2:C:786:LYS:NZ	5:E:72:GLU:CG	2.33	0.90
2:C:786:LYS:HZ1	5:E:72:GLU:CG	1.80	0.89
2:C:662:HIS:HE1	2:C:700:LYS:HD2	1.40	0.87
2:C:783:GLU:CG	5:E:75:TYR:CD2	2.56	0.87
2:C:783:GLU:HG3	5:E:75:TYR:CD2	2.14	0.82
5:E:145:LYS:HB2	5:E:145:LYS:NZ	1.95	0.80
4:A:221:VAL:HG12	5:E:146:GLY:HA3	1.63	0.79
2:C:1180:ARG:CZ	5:E:442:ARG:HA	2.13	0.79
4:A:459:VAL:HG11	4:A:757:ILE:HD13	1.65	0.78
5:E:70:ASP:HB2	5:E:73:ASN:ND2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:221:VAL:HG11	5:E:146:GLY:HA3	1.64	0.77
4:A:264:GLN:HE22	4:A:322:VAL:H	1.31	0.77
5:E:120:MET:HE2	5:E:120:MET:CA	2.12	0.76
2:C:783:GLU:HG2	5:E:75:TYR:CD2	2.20	0.76
2:C:498:MET:HE1	2:C:530:PRO:HB2	1.68	0.76
4:A:486:SER:HB2	4:A:494:VAL:HB	1.68	0.76
2:C:1208:LEU:HB2	2:C:1241:ILE:HD11	1.66	0.76
4:A:221:VAL:CG1	5:E:146:GLY:CA	2.63	0.74
4:A:804:HIS:HD2	4:A:862:TRP:CZ2	2.06	0.74
5:E:149:ASP:N	5:E:149:ASP:OD1	2.20	0.74
4:A:547:CYS:SG	4:A:548:ALA:N	2.61	0.73
4:A:528:ARG:HG3	4:A:530:ASP:H	1.55	0.72
2:C:961:VAL:HA	2:C:964:THR:HG22	1.72	0.71
2:C:1001:VAL:HG12	2:C:1009:MET:HE1	1.71	0.71
4:A:1200:THR:HG22	4:A:1202:PRO:HD2	1.73	0.71
4:A:552:ARG:NH1	4:A:600:GLN:O	2.24	0.70
2:C:655:LYS:NZ	5:E:114:ASP:HB2	2.05	0.70
2:C:963:LYS:HD3	2:C:1003:VAL:HG22	1.73	0.70
4:A:828:GLY:O	4:A:834:LEU:N	2.24	0.70
2:C:568:ARG:NH1	5:E:130:ASP:OD1	2.24	0.69
2:C:783:GLU:OE2	5:E:72:GLU:HG2	1.91	0.69
4:A:507:SER:HB2	4:A:519:VAL:HB	1.73	0.69
2:C:1180:ARG:NH2	5:E:443:LYS:H	1.90	0.69
4:A:1001:ILE:HG13	4:A:1038:LEU:HD21	1.74	0.68
5:E:300:GLY:O	5:E:302:GLY:N	2.21	0.68
2:C:1289:ASN:ND2	2:C:1295:TYR:H	1.93	0.67
4:A:603:ARG:HA	4:A:619:LEU:HB2	1.77	0.66
2:C:662:HIS:HE1	2:C:700:LYS:CD	2.09	0.66
4:A:499:PHE:O	4:A:525:ARG:NH1	2.30	0.65
2:C:622:GLU:OE2	2:C:622:GLU:HA	1.97	0.65
5:E:145:LYS:HB2	5:E:145:LYS:HZ2	1.58	0.65
4:A:550:ASN:ND2	4:A:593:ALA:O	2.30	0.64
4:A:637:PRO:HA	4:A:669:LEU:HA	1.78	0.64
4:A:221:VAL:HG13	5:E:146:GLY:C	2.23	0.64
4:A:558:LEU:HD23	4:A:558:LEU:H	1.63	0.63
2:C:731:LEU:HB3	2:C:750:ILE:HD11	1.80	0.63
2:C:1097:LEU:O	2:C:1100:ASN:ND2	2.32	0.62
2:C:655:LYS:HZ2	5:E:114:ASP:HB2	1.63	0.62
2:C:618:ASP:OD1	2:C:618:ASP:N	2.33	0.62
2:C:621:ASP:OD2	2:C:621:ASP:N	2.30	0.62
5:E:68:ASN:O	5:E:68:ASN:ND2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:947:GLU:HG3	4:A:948:VAL:H	1.65	0.61
2:C:769:VAL:O	2:C:773:LEU:HB2	2.00	0.61
2:C:786:LYS:HZ2	5:E:72:GLU:CD	2.09	0.61
4:A:549:VAL:HG13	4:A:554:VAL:HG22	1.83	0.61
4:A:465:HIS:CE1	4:A:467:GLU:HB2	2.36	0.60
4:A:720:TRP:HA	4:A:733:PRO:HA	1.84	0.60
2:C:581:LEU:HD22	2:C:589:ALA:HB1	1.84	0.60
2:C:974:LEU:HA	2:C:977:VAL:HG12	1.83	0.60
2:C:1001:VAL:O	2:C:1045:ARG:NH2	2.34	0.60
2:C:630:ARG:HH21	5:E:68:ASN:HB2	1.67	0.60
4:A:554:VAL:HG12	4:A:556:ILE:HD11	1.84	0.60
4:A:603:ARG:O	4:A:619:LEU:N	2.34	0.60
2:C:1009:MET:HE2	2:C:1011:PRO:HG2	1.83	0.59
4:A:614:VAL:HG13	4:A:633:LEU:HD21	1.85	0.59
4:A:1083:ASN:N	4:A:1088:LYS:HZ1	2.01	0.58
4:A:553:GLN:HE21	4:A:601:ARG:HB2	1.67	0.58
4:A:511:LEU:HD22	4:A:517:VAL:HG21	1.84	0.58
4:A:1055:VAL:HG23	4:A:1093:MET:HE3	1.85	0.58
4:A:343:LYS:O	4:A:344:THR:OG1	2.17	0.57
4:A:466:ILE:HA	4:A:510:LEU:HD21	1.85	0.57
2:C:972:GLY:O	2:C:976:VAL:HG23	2.04	0.57
5:E:117:GLU:OE1	5:E:117:GLU:HA	2.04	0.57
2:C:513:LYS:HE2	5:E:158:GLU:HG3	1.87	0.57
2:C:570:TYR:O	2:C:574:ILE:HG12	2.04	0.57
2:C:786:LYS:HZ2	5:E:72:GLU:CG	2.17	0.57
4:A:126:LYS:HB2	4:A:128:ARG:HE	1.69	0.57
4:A:946:GLU:OE2	4:A:968:ARG:NH2	2.34	0.57
1:B:25:ASP:OD1	2:C:1259:ARG:NH2	2.30	0.56
2:C:903:GLN:HE21	2:C:906:GLU:HA	1.69	0.56
2:C:1113:THR:HG23	2:C:1150:SER:HA	1.87	0.56
4:A:320:ASP:N	4:A:320:ASP:OD1	2.36	0.56
4:A:545:VAL:HG22	4:A:546:LYS:HE2	1.87	0.56
4:A:617:ILE:HG21	4:A:625:LEU:HD13	1.86	0.56
4:A:464:ARG:HE	4:A:472:ALA:HB1	1.71	0.56
2:C:783:GLU:HG2	5:E:75:TYR:CG	2.41	0.55
4:A:562:GLU:HG2	4:A:582:GLU:HG2	1.88	0.55
2:C:722:GLU:CD	2:C:722:GLU:H	2.15	0.55
2:C:1174:GLU:OE1	2:C:1210:HIS:NE2	2.36	0.55
4:A:640:LEU:HD12	4:A:667:ILE:HD12	1.87	0.55
2:C:1289:ASN:HD22	2:C:1295:TYR:H	1.52	0.55
4:A:278:LEU:HD21	4:A:816:LYS:HG3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:739:LEU:HG	4:A:756:ALA:HB1	1.89	0.54
4:A:565:TYR:HD2	4:A:577:TYR:HB2	1.72	0.54
4:A:428:GLY:HA3	4:A:433:SER:HA	1.89	0.54
2:C:581:LEU:O	2:C:590:ARG:HA	2.07	0.54
2:C:1166:ILE:O	2:C:1170:THR:HG23	2.08	0.54
4:A:456:PRO:HB2	4:A:757:ILE:HG21	1.90	0.54
4:A:544:ILE:HA	4:A:558:LEU:HA	1.89	0.54
2:C:741:LYS:HD3	5:E:76:PHE:HA	1.90	0.54
2:C:834:VAL:O	2:C:838:VAL:HG23	2.08	0.54
2:C:655:LYS:NZ	5:E:115:PRO:HD3	2.22	0.53
4:A:955:PHE:HD1	4:A:995:THR:HG21	1.73	0.53
2:C:729:LYS:HB3	2:C:730:PRO:HD3	1.90	0.53
5:E:300:GLY:C	5:E:302:GLY:H	2.13	0.53
2:C:932:ILE:O	2:C:936:VAL:HG23	2.07	0.53
4:A:438:LEU:HD22	4:A:776:GLN:HB3	1.90	0.53
4:A:474:ILE:HG22	4:A:476:VAL:HG23	1.90	0.53
2:C:565:ASP:O	2:C:568:ARG:HG3	2.08	0.53
4:A:187:MET:HE1	4:A:231:HIS:CE1	2.44	0.53
4:A:555:VAL:HG13	4:A:565:TYR:HA	1.89	0.53
4:A:955:PHE:CD1	4:A:995:THR:HG21	2.43	0.53
5:E:132:LYS:HG3	5:E:132:LYS:O	2.08	0.53
1:B:47:PHE:CZ	4:A:35:GLY:HA3	2.44	0.53
4:A:200:ALA:O	4:A:204:THR:OG1	2.22	0.52
4:A:436:ARG:HH11	4:A:776:GLN:HE22	1.56	0.52
5:E:145:LYS:HB2	5:E:145:LYS:HZ3	1.73	0.52
4:A:443:GLU:CD	4:A:443:GLU:H	2.17	0.52
2:C:1199:VAL:HG11	2:C:1204:CYS:SG	2.49	0.52
2:C:971:MET:HA	2:C:974:LEU:HG	1.91	0.52
4:A:539:PRO:O	4:A:542:LYS:NZ	2.42	0.52
4:A:550:ASN:HB2	4:A:592:LEU:HD11	1.92	0.52
2:C:1179:ASP:O	2:C:1185:ARG:NH1	2.41	0.51
4:A:899:THR:OG1	4:A:900:GLY:N	2.43	0.51
2:C:883:ASP:OD1	2:C:883:ASP:N	2.43	0.51
4:A:1176:GLY:HA2	4:A:1179:CYS:HB2	1.92	0.50
4:A:636:GLN:HG2	4:A:670:GLN:HG2	1.94	0.50
2:C:770:MET:O	2:C:774:ILE:HG12	2.11	0.50
2:C:826:ASP:OD1	2:C:827:ARG:N	2.44	0.50
2:C:746:PHE:O	2:C:750:ILE:HG12	2.12	0.50
2:C:513:LYS:CE	5:E:158:GLU:HG3	2.42	0.50
4:A:553:GLN:HE21	4:A:601:ARG:HD2	1.76	0.49
1:B:58:ASN:O	4:A:856:LYS:NZ	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:812:PRO:HB2	2:C:813:PRO:HD3	1.94	0.49
2:C:1180:ARG:NH1	5:E:442:ARG:HA	2.28	0.49
4:A:512:GLY:H	4:A:515:ALA:HB3	1.77	0.49
2:C:662:HIS:CE1	2:C:700:LYS:CD	2.82	0.49
5:E:133:ARG:C	5:E:133:ARG:CD	2.85	0.49
2:C:741:LYS:HE2	5:E:79:GLU:HB2	1.84	0.49
2:C:1084:ILE:O	2:C:1088:ILE:HG12	2.12	0.49
2:C:700:LYS:HG3	5:E:80:GLU:HG3	1.94	0.49
2:C:903:GLN:NE2	2:C:906:GLU:HA	2.27	0.49
4:A:525:ARG:HG2	4:A:527:ILE:HD11	1.94	0.49
4:A:673:VAL:HA	4:A:690:ARG:HA	1.95	0.49
2:C:622:GLU:OE1	5:E:77:GLU:OE2	2.30	0.49
2:C:661:ARG:NH1	2:C:696:ASP:OD2	2.46	0.48
4:A:404:LEU:HD11	4:A:438:LEU:HD11	1.95	0.48
4:A:849:GLU:HG2	4:A:854:ALA:HA	1.94	0.48
4:A:608:GLY:HA2	4:A:614:VAL:HA	1.96	0.48
4:A:864:SER:HB3	4:A:882:LEU:HD12	1.94	0.48
4:A:550:ASN:ND2	4:A:595:VAL:HG13	2.29	0.48
4:A:716:SER:OG	4:A:717:SER:N	2.46	0.48
2:C:1071:LYS:O	2:C:1075:ARG:HG2	2.14	0.48
4:A:471:ASP:O	4:A:487:ILE:HG21	2.13	0.48
4:A:807:TYR:CE2	4:A:857:ALA:HB3	2.48	0.48
2:C:732:TRP:CZ2	2:C:765:TYR:HB3	2.48	0.48
2:C:810:ILE:O	2:C:813:PRO:HD2	2.14	0.48
4:A:606:ALA:HB3	4:A:642:ILE:HD11	1.95	0.48
4:A:665:LEU:HD21	4:A:667:ILE:HD11	1.96	0.48
4:A:994:GLN:HG2	4:A:1038:LEU:HG	1.96	0.48
2:C:591:VAL:O	2:C:595:GLU:HG3	2.13	0.47
2:C:605:GLY:O	2:C:609:MET:HG2	2.14	0.47
4:A:500:LEU:HB2	4:A:525:ARG:HH22	1.79	0.47
2:C:935:THR:O	2:C:939:ARG:HG2	2.14	0.47
4:A:1201:PRO:HB2	4:A:1202:PRO:HD3	1.96	0.47
5:E:114:ASP:N	5:E:115:PRO:HD2	2.29	0.47
2:C:945:ALA:HA	2:C:948:ARG:HB2	1.95	0.47
4:A:822:GLU:HA	4:A:825:GLU:HG2	1.95	0.47
2:C:648:LEU:HA	2:C:651:VAL:HG12	1.96	0.47
4:A:515:ALA:HA	4:A:528:ARG:HA	1.95	0.47
4:A:642:ILE:HG13	4:A:665:LEU:HD12	1.95	0.47
3:D:26:CYS:HB3	3:D:29:LYS:HE2	1.95	0.47
4:A:137:LYS:O	4:A:137:LYS:HG2	2.15	0.47
4:A:697:ARG:HB2	4:A:717:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:946:LYS:HB3	2:C:946:LYS:HE3	1.68	0.46
2:C:886:HIS:C	2:C:888:LEU:H	2.23	0.46
4:A:48:GLY:HA3	4:A:398:VAL:HG11	1.97	0.46
2:C:495:ARG:O	2:C:495:ARG:NH2	2.43	0.46
2:C:1007:HIS:ND1	2:C:1049:TYR:OH	2.46	0.46
2:C:1187:THR:O	2:C:1191:VAL:HG23	2.14	0.46
2:C:1275:GLY:O	2:C:1276:SER:OG	2.31	0.46
4:A:336:ALA:HA	4:A:351:SER:HA	1.97	0.46
4:A:221:VAL:CG1	5:E:146:GLY:C	2.86	0.46
2:C:908:SER:OG	2:C:912:ASN:ND2	2.49	0.46
2:C:786:LYS:HE2	2:C:828:ARG:HH12	1.81	0.46
5:E:590:GLY:O	5:E:594:GLU:HA	2.16	0.46
2:C:630:ARG:NH2	5:E:68:ASN:CB	2.67	0.46
4:A:581:LYS:HD2	4:A:625:LEU:HD12	1.98	0.46
2:C:575:LEU:O	2:C:579:GLU:HB2	2.16	0.46
2:C:663:THR:O	2:C:667:ILE:HG13	2.16	0.46
4:A:530:ASP:OD2	4:A:530:ASP:N	2.49	0.46
2:C:636:ALA:HB2	2:C:644:LEU:HD22	1.97	0.45
2:C:763:ASN:O	2:C:767:ARG:HG2	2.16	0.45
2:C:735:ILE:HD12	2:C:772:ILE:HD13	1.97	0.45
2:C:1140:GLU:O	2:C:1144:GLN:HG3	2.16	0.45
4:A:477:SER:HA	4:A:482:THR:HA	1.99	0.45
4:A:550:ASN:OD1	4:A:551:GLN:N	2.41	0.45
2:C:911:LEU:HD21	2:C:953:ASP:HB2	1.97	0.45
2:C:925:VAL:HG23	2:C:928:TYR:HB2	1.99	0.45
4:A:579:GLU:OE1	4:A:625:LEU:HG	2.16	0.45
4:A:873:GLN:HG3	4:A:875:ASN:HD22	1.82	0.45
4:A:556:ILE:HG22	4:A:557:ALA:H	1.80	0.45
3:D:29:LYS:HG2	3:D:36:TYR:CZ	2.52	0.45
2:C:1092:ASP:OD2	2:C:1092:ASP:N	2.49	0.45
2:C:1136:TYR:HB2	2:C:1147:VAL:HG11	1.97	0.45
4:A:465:HIS:CE1	4:A:467:GLU:H	2.35	0.45
4:A:587:VAL:HG21	4:A:590:MET:HE3	1.99	0.44
4:A:1009:PHE:HZ	4:A:1046:GLY:HA3	1.81	0.44
2:C:925:VAL:HG23	2:C:928:TYR:HD2	1.81	0.44
2:C:1256:HIS:HD2	2:C:1258:ALA:H	1.65	0.44
2:C:766:THR:O	2:C:770:MET:HB2	2.17	0.44
5:E:133:ARG:CZ	5:E:134:LEU:HB2	2.47	0.44
2:C:630:ARG:CZ	5:E:68:ASN:HB2	2.44	0.44
2:C:783:GLU:HG3	5:E:75:TYR:HD2	1.78	0.44
2:C:855:ASP:OD1	2:C:891:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:663:LEU:HD23	4:A:679:LEU:HB3	1.99	0.44
4:A:318:ASP:O	4:A:319:GLU:C	2.61	0.44
4:A:643:VAL:HG12	4:A:703:ARG:HD3	2.00	0.44
2:C:568:ARG:HH12	5:E:130:ASP:CG	2.25	0.44
2:C:866:LYS:HG3	2:C:909:VAL:HG11	1.99	0.44
4:A:538:THR:HG21	4:A:558:LEU:HD13	1.98	0.44
4:A:620:ASP:OD1	4:A:621:PRO:HD2	2.16	0.44
4:A:1165:SER:OG	4:A:1170:VAL:HG23	2.18	0.44
5:E:145:LYS:O	5:E:145:LYS:HG2	2.17	0.44
4:A:219:HIS:CD2	5:E:148:ARG:HD3	2.52	0.44
4:A:509:SER:HB2	4:A:549:VAL:HG11	2.00	0.44
5:E:70:ASP:HB2	5:E:73:ASN:CG	2.43	0.44
5:E:299:THR:HA	5:E:300:GLY:HA2	1.71	0.44
2:C:1053:ARG:HH22	2:C:1057:ARG:HD2	1.83	0.44
2:C:876:MET:HE2	2:C:876:MET:HB3	1.74	0.43
2:C:721:ILE:HD13	2:C:756:LEU:HB3	2.01	0.43
2:C:804:ASN:O	2:C:808:THR:HG22	2.17	0.43
2:C:623:TYR:O	2:C:627:THR:HG23	2.18	0.43
4:A:745:PHE:HD2	4:A:750:CYS:HB2	1.84	0.43
4:A:1114:SER:HB2	4:A:1215:TYR:CE1	2.53	0.43
2:C:886:HIS:O	2:C:887:LYS:HB3	2.18	0.43
4:A:537:LYS:HE3	4:A:537:LYS:HB2	1.56	0.43
4:A:1104:LEU:HD23	4:A:1119:TYR:HB3	2.01	0.43
2:C:1125:PRO:HG2	2:C:1165:TYR:CE2	2.53	0.43
2:C:904:THR:OG1	2:C:905:THR:N	2.52	0.43
2:C:655:LYS:HZ1	5:E:115:PRO:HD3	1.83	0.43
4:A:618:SER:OG	4:A:628:LEU:HD21	2.19	0.43
4:A:873:GLN:HG3	4:A:875:ASN:ND2	2.33	0.43
2:C:819:TRP:C	2:C:820:GLN:HG2	2.44	0.42
4:A:230:GLU:OE1	4:A:268:ARG:NH2	2.52	0.42
4:A:947:GLU:HG2	4:A:964:GLY:HA3	2.02	0.42
2:C:869:MET:HE1	2:C:896:ILE:HG22	2.01	0.42
4:A:697:ARG:HH11	4:A:717:SER:HA	1.84	0.42
4:A:710:GLU:OE2	4:A:710:GLU:HA	2.19	0.42
2:C:873:GLU:OE1	2:C:912:ASN:HB3	2.20	0.42
5:E:133:ARG:C	5:E:133:ARG:HD2	2.45	0.42
4:A:758:SER:HB2	4:A:763:ARG:HE	1.84	0.42
4:A:980:LYS:HD2	4:A:980:LYS:HA	1.75	0.42
1:B:7:ILE:HG13	3:D:8:LEU:O	2.19	0.42
2:C:806:ILE:HG12	2:C:810:ILE:HD12	2.00	0.42
2:C:1025:LYS:HA	2:C:1025:LYS:HD2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:32:VAL:HG22	4:A:39:GLU:HB3	2.00	0.42
2:C:1053:ARG:CZ	2:C:1053:ARG:HB3	2.49	0.42
4:A:1035:THR:HG22	4:A:1047:ALA:HB3	2.00	0.42
4:A:370:GLU:OE2	4:A:390:ARG:HD3	2.18	0.42
2:C:641:ILE:HD11	2:C:675:MET:SD	2.60	0.42
2:C:1260:LYS:HA	2:C:1260:LYS:HD3	1.84	0.42
2:C:568:ARG:NH2	5:E:130:ASP:OD1	2.53	0.42
2:C:774:ILE:O	2:C:777:PHE:HB2	2.19	0.42
2:C:1009:MET:HG2	2:C:1011:PRO:HD2	2.02	0.42
2:C:1289:ASN:HD21	2:C:1296:ILE:H	1.68	0.42
4:A:267:ILE:HD13	4:A:322:VAL:HG12	2.01	0.42
4:A:1214:ARG:HG2	4:A:1215:TYR:CE2	2.55	0.42
4:A:743:SER:OG	4:A:744:GLY:O	2.38	0.41
2:C:732:TRP:O	2:C:735:ILE:HG13	2.19	0.41
2:C:811:LEU:HD22	2:C:815:PHE:HE2	1.84	0.41
2:C:929:LEU:N	2:C:930:PRO:HD2	2.35	0.41
2:C:1110:VAL:O	2:C:1114:VAL:HG23	2.19	0.41
4:A:629:SER:OG	4:A:681:PRO:O	2.38	0.41
4:A:821:GLU:O	4:A:824:VAL:HG12	2.19	0.41
4:A:858:GLY:HA3	4:A:861:GLN:HG3	2.03	0.41
1:B:32:LEU:HD11	2:C:1287:ILE:HG21	2.02	0.41
2:C:631:ALA:O	2:C:635:VAL:HG12	2.20	0.41
2:C:814:PHE:O	2:C:818:PHE:HB2	2.20	0.41
2:C:1070:LYS:NZ	2:C:1070:LYS:HB3	2.36	0.41
4:A:947:GLU:HG3	4:A:948:VAL:N	2.33	0.41
4:A:1018:GLU:N	4:A:1018:GLU:OE2	2.52	0.41
4:A:638:GLU:HG3	4:A:670:GLN:HB3	2.02	0.41
2:C:1180:ARG:NH2	5:E:442:ARG:HA	2.35	0.41
2:C:1250:CYS:SG	2:C:1269:TYR:HB2	2.60	0.41
4:A:172:GLY:O	4:A:237:THR:OG1	2.30	0.41
4:A:472:ALA:O	4:A:487:ILE:HG22	2.20	0.41
2:C:551:LEU:O	2:C:555:VAL:HG23	2.20	0.41
4:A:895:ARG:HG2	4:A:902:ASP:O	2.21	0.41
1:B:57:GLU:O	1:B:59:GLU:N	2.53	0.41
2:C:641:ILE:N	2:C:642:PRO:HD2	2.35	0.41
2:C:745:ALA:HB2	5:E:76:PHE:CE1	2.55	0.41
2:C:776:GLU:O	2:C:779:SER:HB3	2.21	0.41
2:C:1014:LYS:H	2:C:1014:LYS:HE2	1.84	0.41
2:C:1141:LEU:C	2:C:1143:VAL:H	2.29	0.41
4:A:451:GLU:HG3	4:A:760:ASN:O	2.21	0.41
5:E:134:LEU:HD12	5:E:134:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1193:GLN:HB2	2:C:1233:ALA:HA	2.02	0.41
4:A:761:THR:HG22	4:A:762:LEU:H	1.85	0.41
3:D:22:LEU:HG	3:D:69:ALA:HB2	2.03	0.41
4:A:168:TYR:HB2	4:A:185:LEU:HB2	2.03	0.41
3:D:59:VAL:HG13	3:D:87:LYS:HA	2.02	0.41
4:A:423:LEU:HB2	4:A:438:LEU:HB2	2.03	0.40
2:C:856:ASP:HB3	2:C:864:TYR:CE2	2.57	0.40
2:C:925:VAL:HG23	2:C:928:TYR:CD2	2.56	0.40
2:C:943:LYS:HB3	2:C:947:VAL:HG21	2.02	0.40
2:C:955:ILE:HD13	2:C:974:LEU:HD13	2.03	0.40
4:A:521:PRO:HA	4:A:544:ILE:HB	2.02	0.40
2:C:514:ALA:O	2:C:518:GLN:HG3	2.21	0.40
2:C:583:ILE:HD13	2:C:627:THR:HG22	2.02	0.40
2:C:772:ILE:HG23	2:C:775:ARG:HH21	1.86	0.40
2:C:849:ILE:O	2:C:853:ILE:HG12	2.21	0.40
2:C:1055:TRP:CE3	2:C:1055:TRP:HA	2.56	0.40
3:D:49:CYS:HB3	3:D:87:LYS:HD3	2.02	0.40
4:A:618:SER:CB	4:A:628:LEU:HD21	2.51	0.40
2:C:766:THR:HA	2:C:769:VAL:HG12	2.03	0.40
2:C:783:GLU:OE2	2:C:786:LYS:HE3	2.21	0.40
4:A:34:ARG:H	4:A:34:ARG:HG2	1.75	0.40
4:A:492:GLU:N	4:A:492:GLU:OE1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	76/86 (88%)	75 (99%)	1 (1%)	0	100	100
2	C	813/872 (93%)	784 (96%)	29 (4%)	0	100	100
3	D	91/110 (83%)	86 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1165/1250 (93%)	1088 (93%)	76 (6%)	1 (0%)	48 70
5	E	474/958 (50%)	459 (97%)	12 (2%)	3 (1%)	21 42
All	All	2619/3276 (80%)	2492 (95%)	123 (5%)	4 (0%)	44 66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	301	SER
5	E	595	LYS
5	E	275	GLN
4	A	234	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	69/77 (90%)	65 (94%)	4 (6%)	18 39
2	C	701/753 (93%)	666 (95%)	35 (5%)	22 46
3	D	80/95 (84%)	77 (96%)	3 (4%)	29 56
4	A	1020/1071 (95%)	940 (92%)	80 (8%)	11 26
5	E	51/787 (6%)	39 (76%)	12 (24%)	1 1
All	All	1921/2783 (69%)	1787 (93%)	134 (7%)	16 31

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	ILE
1	B	21	THR
1	B	32	LEU
1	B	50	LEU
2	C	500	LEU
2	C	560	LEU
2	C	576	VAL

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Mol	Chain	Res	Type
2	C	582	LEU
2	C	617	ILE
2	C	618	ASP
2	C	621	ASP
2	C	635	VAL
2	C	654	SER
2	C	655	LYS
2	C	683	LEU
2	C	700	LYS
2	C	722	GLU
2	C	754	ILE
2	C	756	LEU
2	C	760	GLU
2	C	779	SER
2	C	792	VAL
2	C	828	ARG
2	C	857	LEU
2	C	870	GLU
2	C	902	GLU
2	C	905	THR
2	C	906	GLU
2	C	931	GLN
2	C	949	GLN
2	C	956	SER
2	C	993	ILE
2	C	1048	GLU
2	C	1070	LYS
2	C	1092	ASP
2	C	1100	ASN
2	C	1101	LEU
2	C	1123	CYS
2	C	1271	SER
3	D	26	CYS
3	D	35	SER
3	D	97	ASP
4	A	8	LEU
4	A	12	THR
4	A	64	SER
4	A	152	LEU
4	A	156	SER
4	A	171	VAL
4	A	229	GLU

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Mol	Chain	Res	Type
4	A	252	SER
4	A	278	LEU
4	A	295	THR
4	A	296	LYS
4	A	297	SER
4	A	326	ARG
4	A	351	SER
4	A	364	LEU
4	A	367	ASP
4	A	374	SER
4	A	390	ARG
4	A	435	LEU
4	A	450	SER
4	A	452	LEU
4	A	465	HIS
4	A	469	GLU
4	A	477	SER
4	A	491	VAL
4	A	503	THR
4	A	516	LEU
4	A	520	TYR
4	A	530	ASP
4	A	538	THR
4	A	541	LYS
4	A	543	THR
4	A	546	LYS
4	A	547	CYS
4	A	576	GLU
4	A	578	THR
4	A	587	VAL
4	A	588	VAL
4	A	591	SER
4	A	592	LEU
4	A	599	GLU
4	A	618	SER
4	A	640	LEU
4	A	641	CYS
4	A	665	LEU
4	A	677	THR
4	A	685	ASP
4	A	689	THR
4	A	713	LEU

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Mol	Chain	Res	Type
4	A	734	LEU
4	A	743	SER
4	A	750	CYS
4	A	761	THR
4	A	767	LEU
4	A	770	LEU
4	A	775	ASN
4	A	776	GLN
4	A	805	ASN
4	A	824	VAL
4	A	864	SER
4	A	865	VAL
4	A	873	GLN
4	A	890	SER
4	A	897	SER
4	A	899	THR
4	A	920	VAL
4	A	959	VAL
4	A	984	LYS
4	A	986	ILE
4	A	994	GLN
4	A	995	THR
4	A	1020	GLN
4	A	1066	VAL
4	A	1103	SER
4	A	1133	THR
4	A	1137	ASP
4	A	1151	GLU
4	A	1170	VAL
4	A	1184	SER
4	A	1217	PHE
5	E	68	ASN
5	E	70	ASP
5	E	79	GLU
5	E	116	LEU
5	E	120	MET
5	E	126	GLN
5	E	133	ARG
5	E	145	LYS
5	E	148	ARG
5	E	149	ASP
5	E	155	ASP

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Mol	Chain	Res	Type
5	E	162	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	35	GLN
2	C	599	ASN
2	C	662	HIS
2	C	737	GLN
2	C	738	HIS
2	C	794	GLN
2	C	829	ASN
2	C	863	GLN
2	C	891	GLN
2	C	903	GLN
2	C	941	ASN
2	C	1002	ASN
2	C	1028	HIS
2	C	1104	GLN
2	C	1108	ASN
2	C	1134	ASN
2	C	1184	HIS
2	C	1228	GLN
2	C	1256	HIS
2	C	1289	ASN
2	C	1293	ASN
3	D	78	GLN
4	A	138	GLN
4	A	218	ASN
4	A	219	HIS
4	A	254	ASN
4	A	264	GLN
4	A	307	GLN
4	A	417	ASN
4	A	465	HIS
4	A	551	GLN
4	A	553	GLN
4	A	749	GLN
4	A	776	GLN
4	A	796	ASN
4	A	804	HIS

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Mol	Chain	Res	Type
4	A	805	ASN
4	A	870	ASN
4	A	873	GLN
4	A	875	ASN
4	A	916	ASN
4	A	1017	ASN
4	A	1052	ASN
4	A	1094	ASN
4	A	1181	GLN
5	E	68	ASN
5	E	167	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

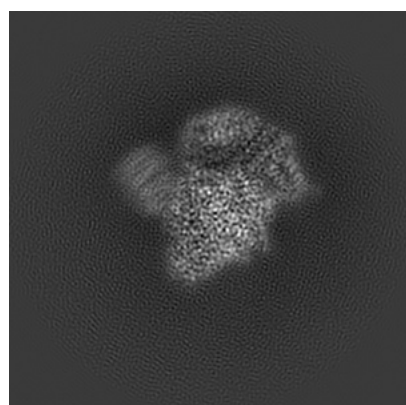
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31330. These allow visual inspection of the internal detail of the map and identification of artifacts.

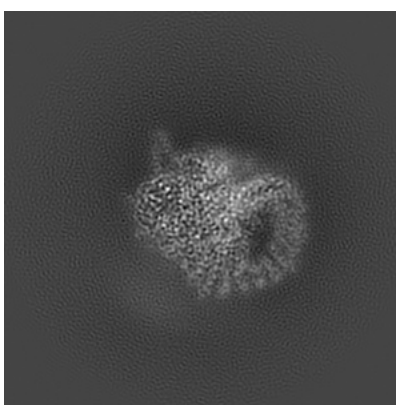
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

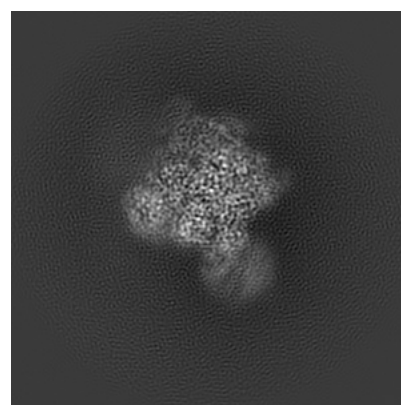
6.1.1 Primary map



X



Y

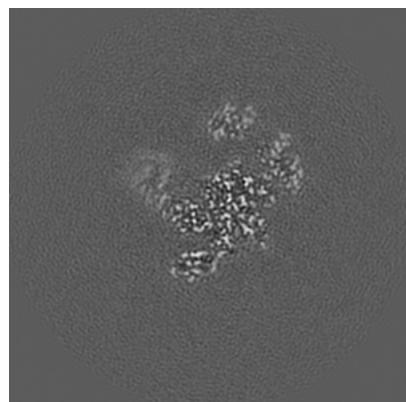


Z

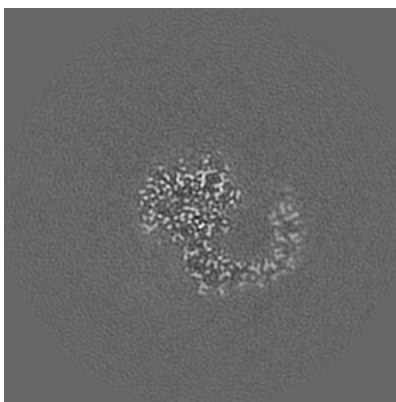
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

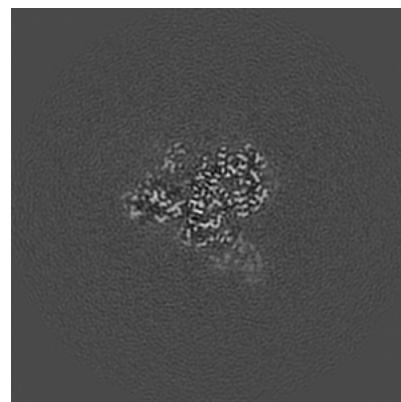
6.2.1 Primary map



X Index: 120



Y Index: 120

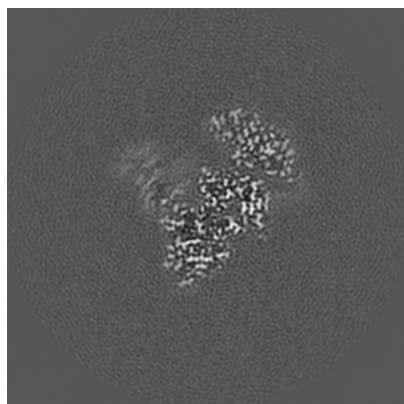


Z Index: 120

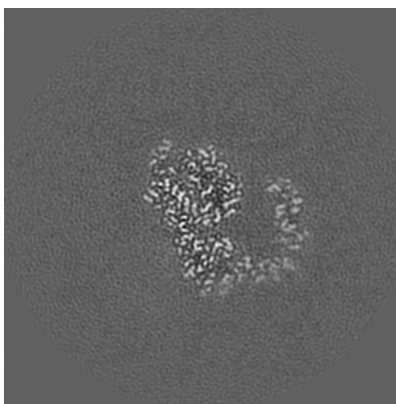
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

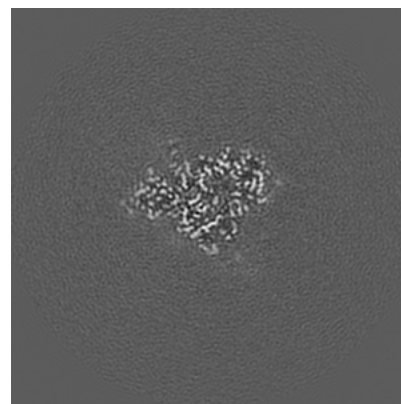
6.3.1 Primary map



X Index: 127



Y Index: 127

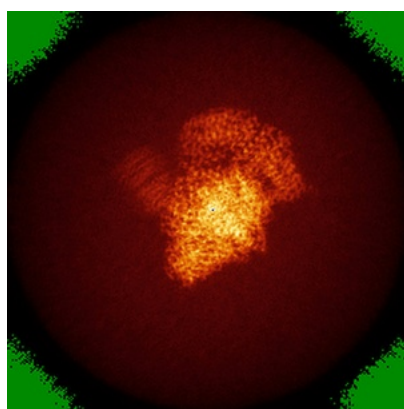


Z Index: 116

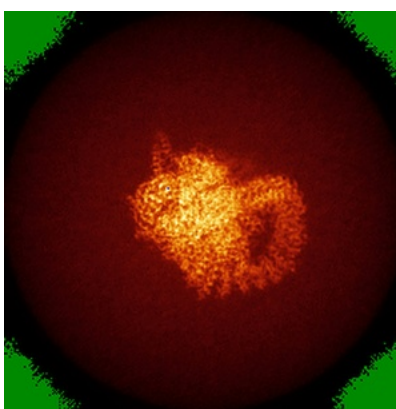
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

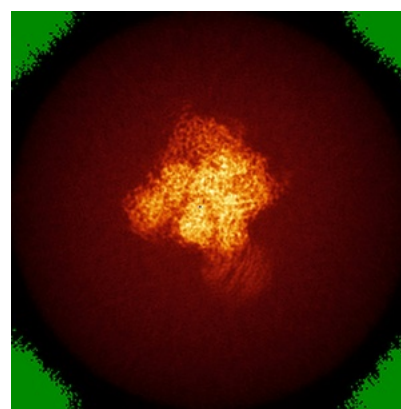
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

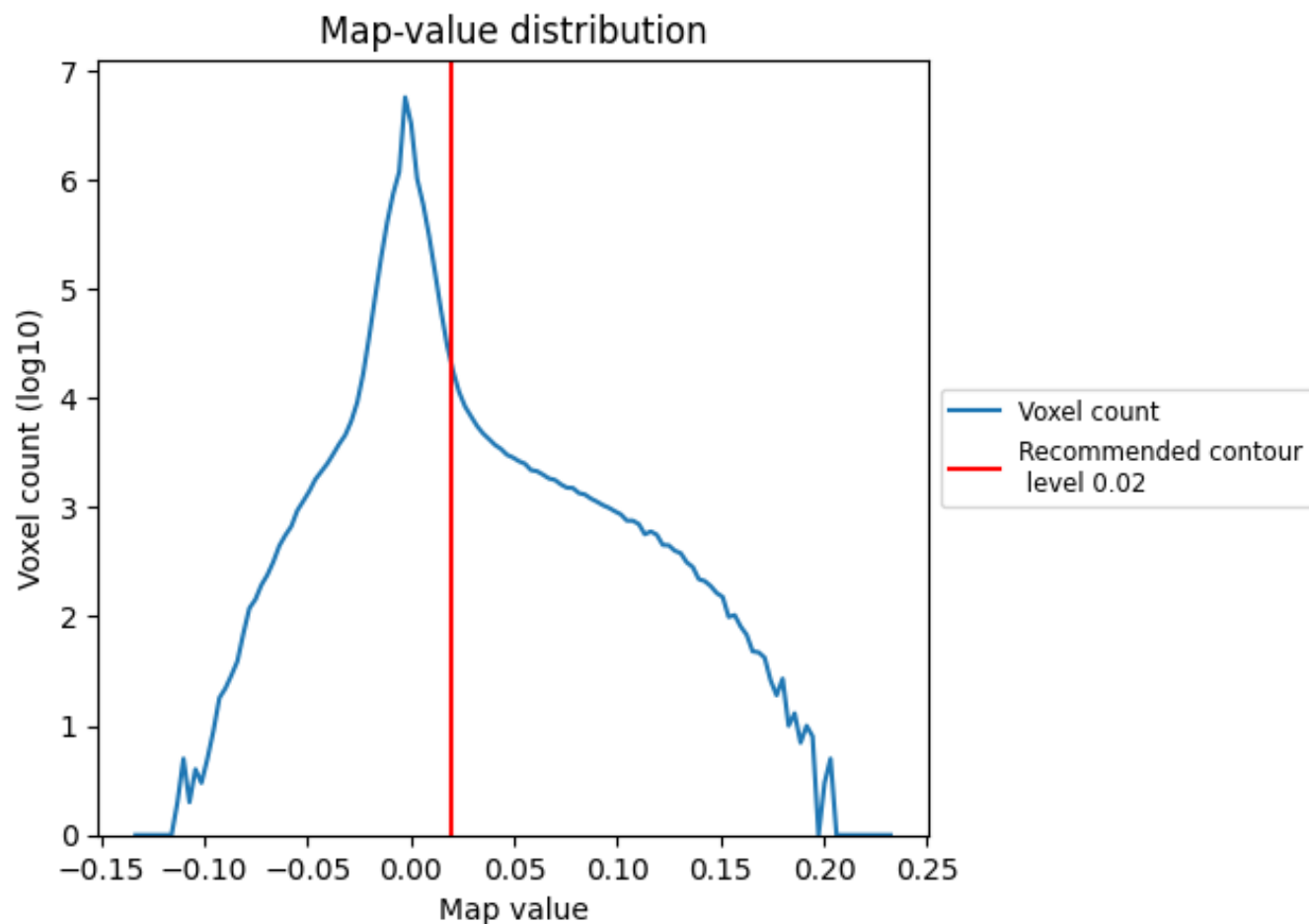
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

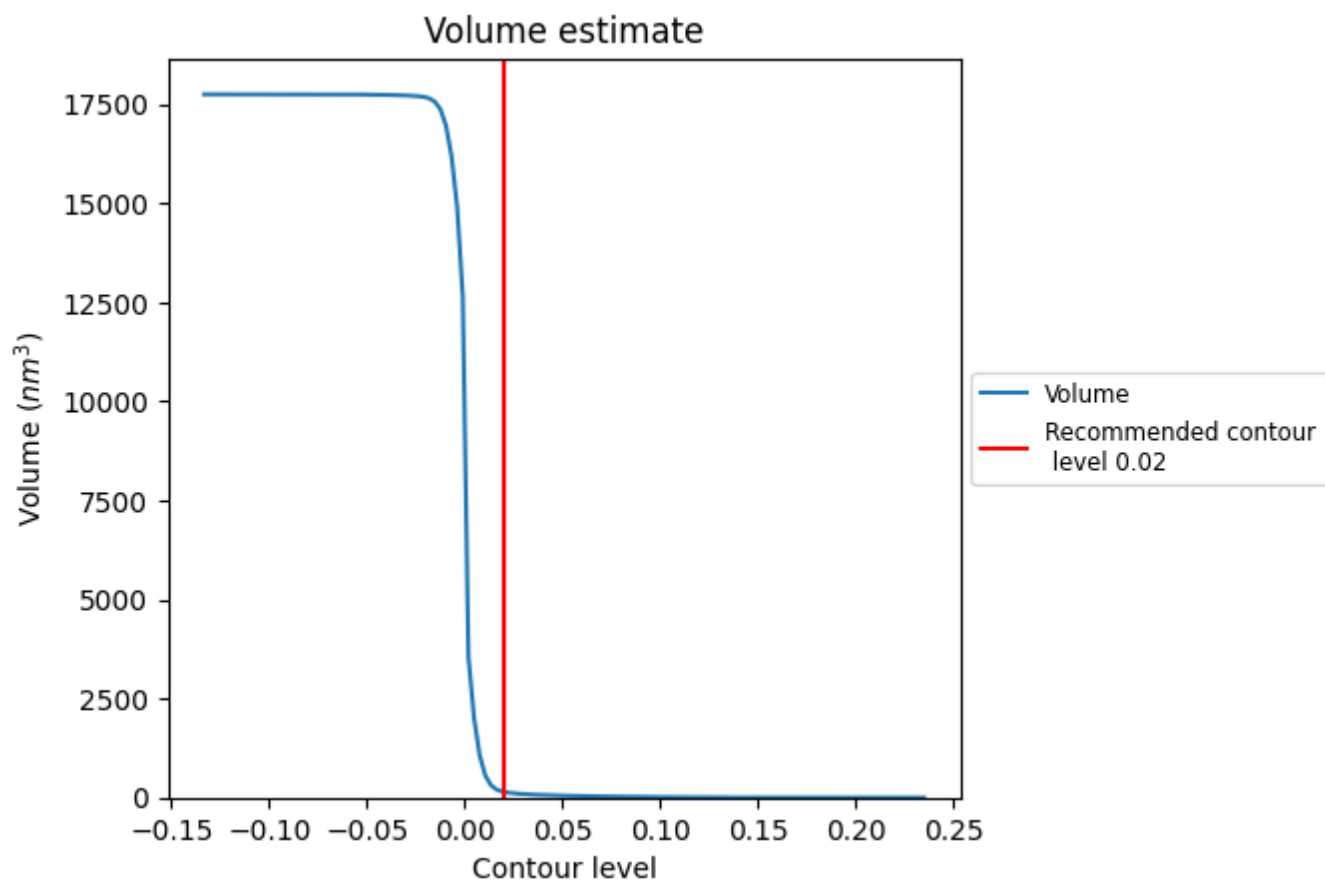
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

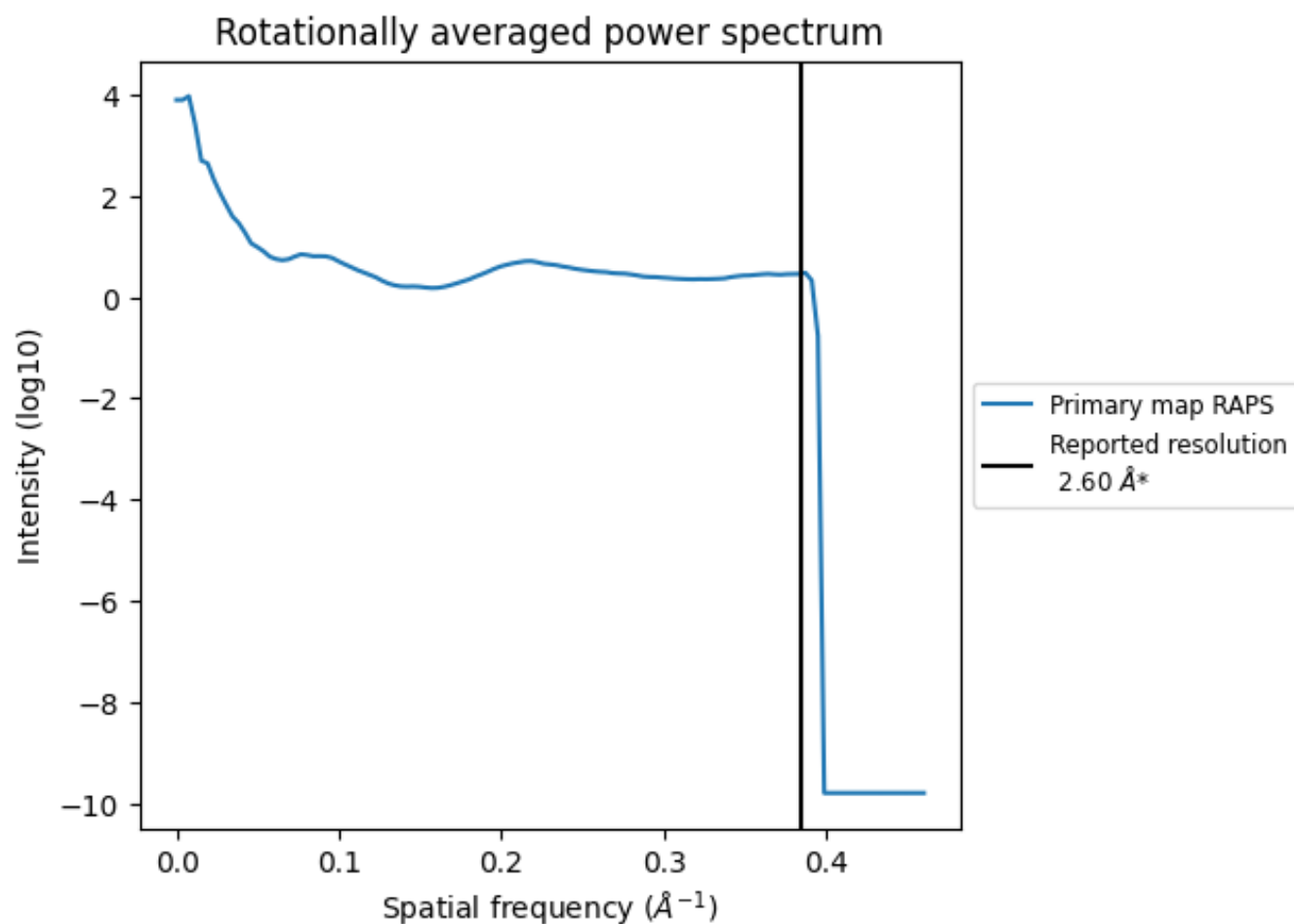
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 145 nm³; this corresponds to an approximate mass of 131 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.385 $\text{\AA}^{-1}$

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

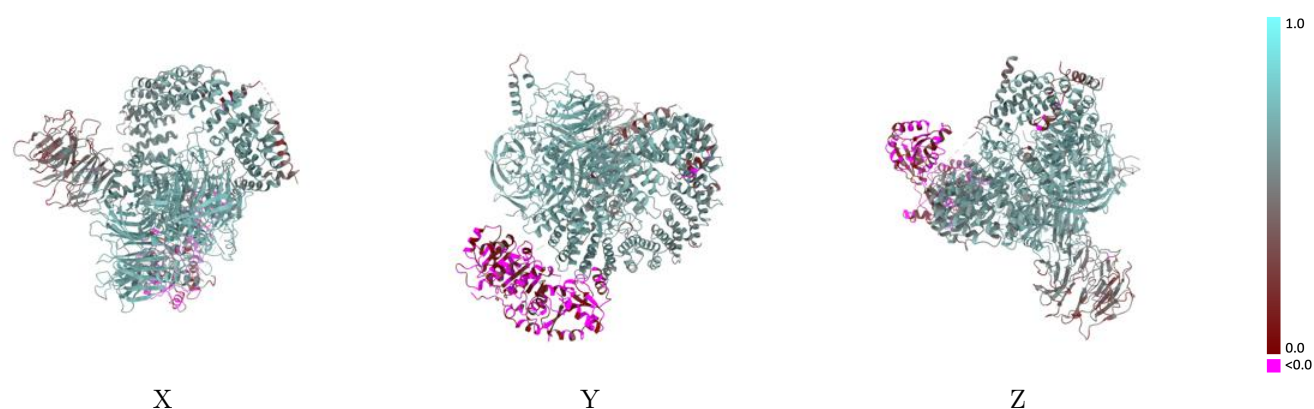
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-31330 and PDB model 7EVN. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

9.2 Q-score mapped to coordinate model [i](#)

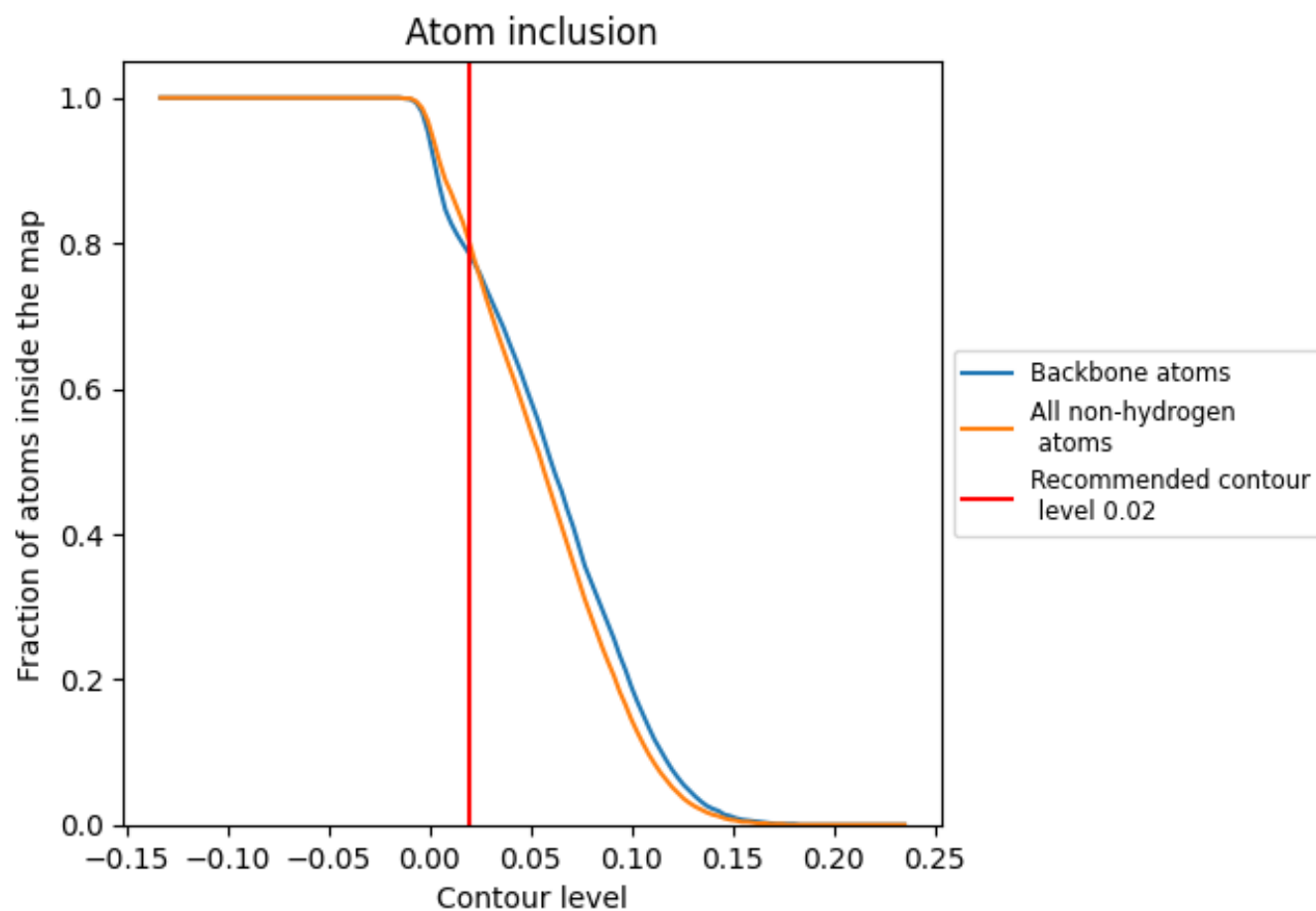


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7990	0.5400
A	0.8870	0.6040
B	0.9840	0.6760
C	0.9300	0.6110
D	0.9240	0.6470
E	0.0950	0.0770

